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Structure of molecules in crystalline lattice obtained by a modified method of molecular mechanics: Calculations of 13C chemical shifts

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Abstract

A program for the calculation of the geometric structure of molecular crystals on the basis of the methods of molecular mechanics (MM) has been developed. A standard MM method has been modified by including force fields taking into account the specific (H-bond and van der Waals) interactions and the periodicity of the crystal lattice of an arbitrary form and symmetry. The geometric parameters of the molecule in a crystal calculated by this method are in agreement with the experimental X-ray data within reasonable accuracy. The nuclear magnetic resonance 13C chemical shifts have been calculated for the molecular geometry obtained by the quantum chemical UB3LYP/6-31G(d, p) method. The results of the calculations have been used to explain some unusual NMR spectral data.